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# (2,2′-Bipyridyl)bis[*N*-(2-hydroxyethyl)-*N*-*n*-propyldithiocarbamato-$\kappa^2 S,S'$]-cadmium(II) acetonitrile solvate

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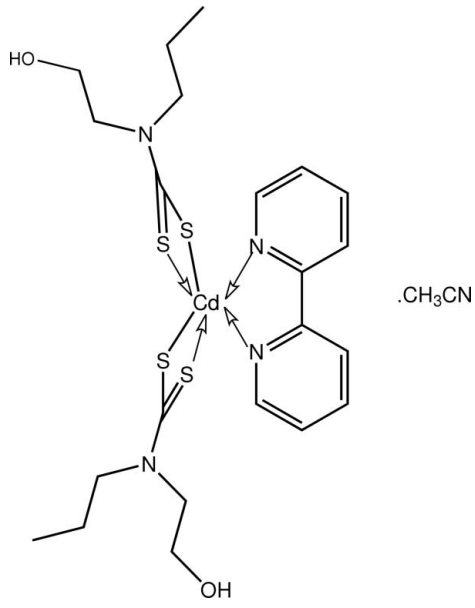
Key indicators: single-crystal X-ray study; $T$ = 98 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.030; $wR$ factor = 0.080; data-to-parameter ratio = 18.3.

The title complex, $[Cd(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot CH_3CN$, features a distorted octahedral $N_2S_4$ geometry for the $Cd^{II}$ centre defined by a pair of asymmetrically chelating dithiocarbamate ligands as well as a 2,2′-bipyridine ligand. Supramolecular chains along [001] are formed in the crystal structure, mediated by O—H···S hydrogen bonds; the acetonitrile solvent molecules are associated with the chains *via* O—H···N hydrogen bonds.

## Related literature

For background to supramolecular polymers of zinc-triad 1,1-dithiolates, see: Tiekink (2003); Lai *et al.* (2002); Chen *et al.* (2006); Benson *et al.* (2007). For the synthesis, see: Lai & Tiekink (2004).




## Experimental

### Crystal data

$[Cd(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot C_2H_3N$
$M_r$ = 666.21
Monoclinic, $P2_1/c$
$a$ = 7.3277 (7) Å
$b$ = 23.822 (2) Å
$c$ = 17.1159 (18) Å
$\beta$ = 99.786 (1)°
$V$ = 2944.2 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.06 mm$^{-1}$
$T$ = 98 K
0.36 × 0.22 × 0.11 mm

### Data collection

Rigaku AFC12K/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min}$ = 0.828, $T_{max}$ = 1
18201 measured reflections
6043 independent reflections
5711 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.027

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.080
$S$ = 1.09
6043 reflections
331 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.69 e Å$^{-3}$

**Table 1**
Selected bond lengths (Å).

| | | | |
|---|---|---|---|
| Cd—N3 | 2.361 (2) | Cd—S3 | 2.6539 (7) |
| Cd—N4 | 2.406 (2) | Cd—S4 | 2.6704 (7) |
| Cd—S1 | 2.5872 (7) | Cd—S2 | 2.7816 (7) |

**Table 2**
Hydrogen-bond geometry (Å, °).

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1o···N5 | 0.84 | 2.06 | 2.898 (3) | 174 |
| O2—H2o···S2$^{i}$ | 0.84 | 2.55 | 3.388 (2) | 175 |

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *PATTY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5240).

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# supporting information

*Acta Cryst.* (2009). E**65**, m1669–m1670 [doi:10.1107/S1600536809049666]

# (2,2′-Bipyridyl)bis[*N*-(2-hydroxyethyl)-*N*-*n*-propyldithiocarbamato-$\kappa^2 S,S'$]cadmium(II) acetonitrile solvate

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## S1. Comment

Crystal engineering studies on the zinc-triad 1,1-dithiolates have generated 1-D, 2-D and 3-D architectures (Lai *et al.*, 2002; Tiekink, 2003; Chen *et al.*, 2006), in particular with dithiocarbamate ligands functionalized with hydrogen-bonding capacity (Benson *et al.*, 2007). As a continuation of studies in this field, the structure of the title compound, (I), was investigated.

The molecular structure of (I) features a hexa-coordinated $Cd^{II}$ centre defined by two asymmetrically chelating dithiocarbamate ligands (Cd–S1, S2 = 2.5872 (7) and 2.7816 (7) Å, and Cd–S3, S4 = 2.6539 (7) and 2.6704 (7) Å) and a chelating 2,2′-bipyridyl ligand (Cd–N3, N4 = 2.361 (2), 2.406 (2) Å). The resulting $N_2S_4$ donor set defines a distorted octahedral geometry.

The crystal packing is dominated by O–H···O and O–H···N hydrogen bonds, Table 1. The latter involve the O1-hydroxyl group and the nitrile-N5 atom of the solvent acetonitrile molecule. The O2-hydroxyl group forms hydrogen bonds with the dithiocarbamate-S2 atom to generate a supramolecular chain along [0 0 1], Table 1 and Fig. 2.

## S2. Experimental

Compound (I) was prepared following the standard literature procedure from the reaction of $Cd[S_2CN(CH_2CH_2OH)(n\text{-}Pr)]_2$ and 2,2′-bipyridyl (Lai & Tiekink, 2004). Colourless crystals were obtained from the slow evaporation of an acetonitrile solution of (I). IR (KBr, $cm^{-1}$): 1471 (*m*) *v*(C=N); 1183 (*s*) *v*(C—S).

## S3. Refinement

C-bound H-atoms were placed in calculated positions (C–H 0.95–0.99 Å) and were included in the refinement in the riding model approximation with $U_{iso}$(H) set to 1.2$U_{eq}$(C). A rotating group model was used for the methyl groups. The O-bound H-atoms were located in a difference Fourier map and each refined with an O–H restraint of 0.840±0.001 Å, and with $U_{iso}$(H) = 1.5$U_{eq}$(carrier atom).

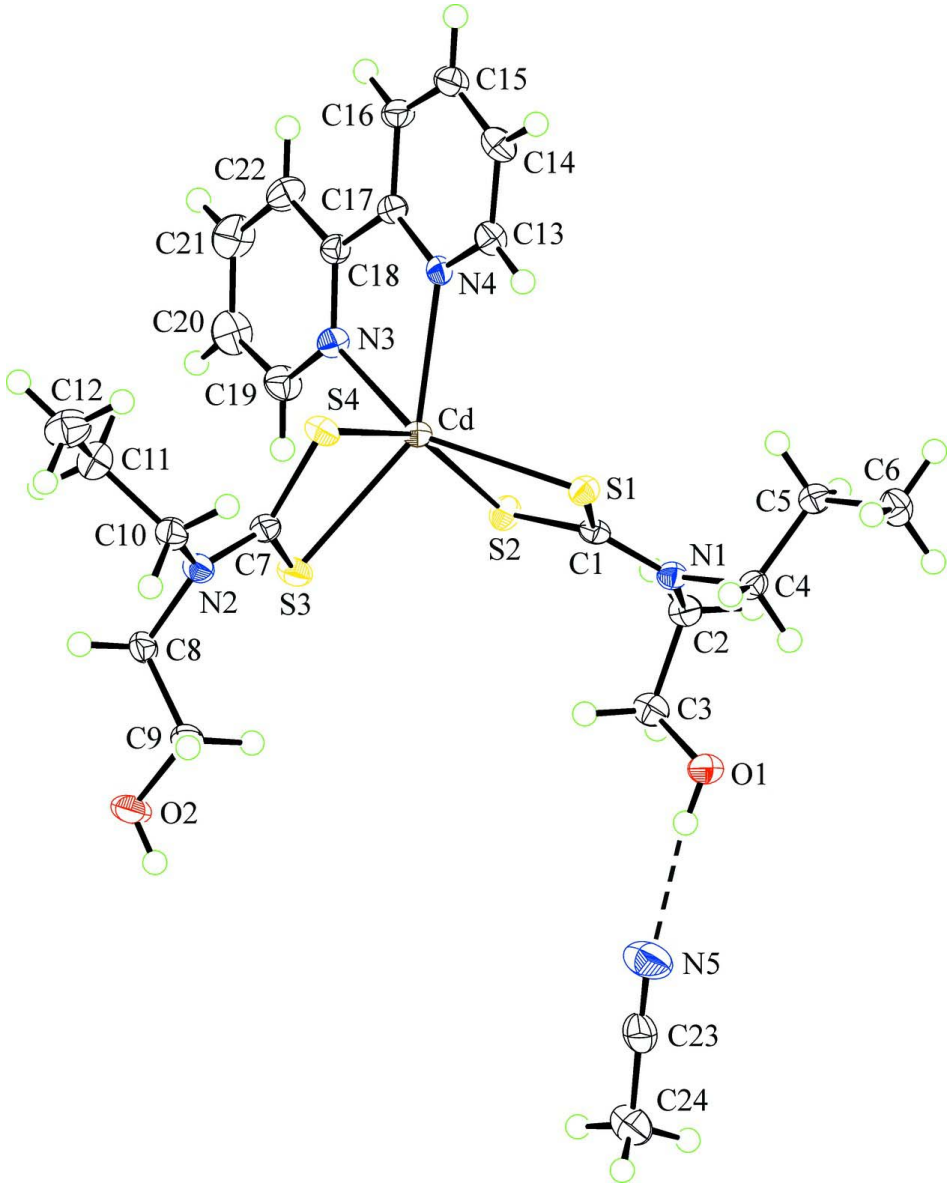


**Figure 1**

Molecular structure of (I) showing displacement ellipsoids at the 50% probability level. The O–H···N hydrogen bond is shown as a dashed line.

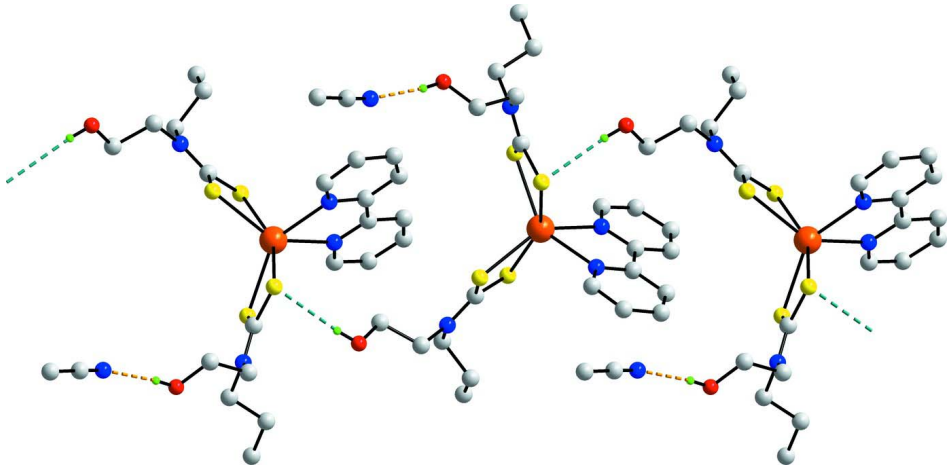

**Figure 2**

Supramolecular chain in (I) mediated by O–H···S (green dashed lines) hydrogen bonds. The solvent acetonitrile molecules are connected by O–H···N hydrogen bonds (orange dashed lines). Hydrogen atoms not involved in the hydrogen bonding are omitted for reasons of clarity. Colour code: Cd, orange; S, yellow; O, red; N, blue; C, grey; and H, green.

**(2,2′-Bipyridyl)bis[*N*-(2-hydroxyethyl)-*N*-*n*- propyldithiocarbamato-$\kappa^2S,S'$]cadmium(II) acetonitrile solvate**

*Crystal data*

$[Cd(C_6H_{12}NOS_2)_2(C_{10}H_8N_2)]\cdot C_2H_3N$
$M_r = 666.21$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.3277\ (7)$ Å
$b = 23.822\ (2)$ Å
$c = 17.1159\ (18)$ Å
$\beta = 99.786\ (1)°$
$V = 2944.2\ (5)$ Å$^3$
$Z = 4$
$F(000) = 1368$
$D_x = 1.503$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 18141 reflections
$\theta = 2.1–40.6°$
$\mu = 1.06$ mm$^{-1}$
$T = 98$ K
Block, colourless
0.36 × 0.22 × 0.11 mm

*Data collection*

Rigaku AFC12K/SATURN724 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.828$, $T_{max} = 1$
18201 measured reflections
6043 independent reflections
5711 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$
$\theta_{max} = 26.5°$, $\theta_{min} = 2.1°$
$h = -9\rightarrow9$
$k = -25\rightarrow29$
$l = -21\rightarrow21$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.080$
$S = 1.09$
6043 reflections
331 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0396P)^2 + 3.165P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 0.70$ e Å$^{-3}$
$\Delta\rho_{min} = -0.69$ e Å$^{-3}$

*Special details*

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement**. Refinement of $F^2$ against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on $F^2$, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative $F^2$. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on $F^2$ are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd | 0.22264 (2) | 0.757722 (7) | 0.046853 (9) | 0.01758 (7) |
| S1 | 0.17585 (8) | 0.85953 (3) | 0.09227 (3) | 0.01984 (13) |
| S2 | 0.54757 (9) | 0.82033 (3) | 0.06550 (4) | 0.02253 (13) |
| S3 | 0.35255 (9) | 0.69177 (3) | 0.16861 (4) | 0.02338 (14) |
| S4 | −0.04308 (9) | 0.69484 (3) | 0.09167 (3) | 0.02234 (13) |
| O1 | 0.7384 (3) | 0.95516 (8) | 0.26074 (11) | 0.0274 (4) |
| H1O | 0.8084 | 0.9465 | 0.3031 | 0.041* |
| O2 | 0.4126 (3) | 0.60342 (9) | 0.39861 (11) | 0.0356 (5) |
| H2O | 0.4471 | 0.6205 | 0.4415 | 0.053* |
| N1 | 0.4822 (3) | 0.92222 (9) | 0.11936 (11) | 0.0184 (4) |
| N2 | 0.0887 (3) | 0.62810 (9) | 0.21271 (12) | 0.0215 (4) |
| N3 | 0.3447 (3) | 0.70592 (9) | −0.04998 (12) | 0.0205 (4) |
| N4 | 0.0208 (3) | 0.76057 (8) | −0.07961 (12) | 0.0177 (4) |
| N5 | 0.9711 (4) | 0.93255 (13) | 0.41198 (16) | 0.0471 (8) |
| C1 | 0.4102 (3) | 0.87219 (10) | 0.09512 (13) | 0.0183 (5) |
| C2 | 0.6792 (3) | 0.93562 (11) | 0.12198 (14) | 0.0212 (5) |
| H2A | 0.6918 | 0.9762 | 0.1116 | 0.025* |
| H2B | 0.7258 | 0.9146 | 0.0795 | 0.025* |
| C3 | 0.7967 (4) | 0.92111 (12) | 0.20105 (15) | 0.0250 (5) |
| H3A | 0.7818 | 0.8809 | 0.2132 | 0.030* |
| H3B | 0.9290 | 0.9282 | 0.1991 | 0.030* |
| C4 | 0.3645 (3) | 0.96886 (10) | 0.13808 (13) | 0.0195 (5) |
| H4A | 0.4397 | 0.9948 | 0.1758 | 0.023* |
| H4B | 0.2640 | 0.9538 | 0.1640 | 0.023* |
| C5 | 0.2802 (4) | 1.00116 (11) | 0.06364 (14) | 0.0218 (5) |
| H5A | 0.3806 | 1.0175 | 0.0388 | 0.026* |
| H5B | 0.2086 | 0.9750 | 0.0251 | 0.026* |
| C6 | 0.1535 (4) | 1.04789 (12) | 0.08326 (16) | 0.0263 (5) |
| H6A | 0.1014 | 1.0680 | 0.0346 | 0.039* |
| H6B | 0.2248 | 1.0741 | 0.1207 | 0.039* |
| H6C | 0.0530 | 1.0317 | 0.1071 | 0.039* |
| C7 | 0.1289 (3) | 0.66779 (11) | 0.16308 (14) | 0.0198 (5) |

| | | | | |
|---|---|---|---|---|
| C8 | 0.2339 (4) | 0.60092 (11) | 0.27098 (14) | 0.0227 (5) |
| H8A | 0.3515 | 0.6003 | 0.2498 | 0.027* |
| H8B | 0.1977 | 0.5616 | 0.2792 | 0.027* |
| C9 | 0.2634 (4) | 0.63157 (12) | 0.34969 (14) | 0.0241 (5) |
| H9A | 0.2952 | 0.6714 | 0.3424 | 0.029* |
| H9B | 0.1500 | 0.6300 | 0.3739 | 0.029* |
| C10 | −0.1000 (4) | 0.60685 (11) | 0.21058 (15) | 0.0232 (5) |
| H10A | −0.1895 | 0.6373 | 0.1930 | 0.028* |
| H10B | −0.1155 | 0.5956 | 0.2648 | 0.028* |
| C11 | −0.1435 (4) | 0.55671 (12) | 0.15499 (17) | 0.0293 (6) |
| H11A | −0.1319 | 0.5680 | 0.1004 | 0.035* |
| H11B | −0.0530 | 0.5264 | 0.1717 | 0.035* |
| C12 | −0.3363 (4) | 0.53524 (15) | 0.15584 (18) | 0.0370 (7) |
| H12A | −0.3612 | 0.5032 | 0.1198 | 0.056* |
| H12B | −0.4261 | 0.5651 | 0.1386 | 0.056* |
| H12C | −0.3472 | 0.5235 | 0.2097 | 0.056* |
| C13 | −0.1430 (3) | 0.78695 (11) | −0.09045 (15) | 0.0223 (5) |
| H13 | −0.1766 | 0.8074 | −0.0474 | 0.027* |
| C14 | −0.2656 (4) | 0.78577 (12) | −0.16151 (16) | 0.0267 (6) |
| H14 | −0.3805 | 0.8051 | −0.1672 | 0.032* |
| C15 | −0.2165 (4) | 0.75569 (11) | −0.22421 (16) | 0.0267 (6) |
| H15 | −0.2978 | 0.7540 | −0.2737 | 0.032* |
| C16 | −0.0475 (4) | 0.72821 (11) | −0.21382 (14) | 0.0230 (5) |
| H16 | −0.0107 | 0.7078 | −0.2562 | 0.028* |
| C17 | 0.0676 (3) | 0.73098 (10) | −0.14026 (14) | 0.0179 (5) |
| C18 | 0.2499 (3) | 0.70174 (10) | −0.12429 (14) | 0.0193 (5) |
| C19 | 0.5105 (4) | 0.68052 (12) | −0.03162 (16) | 0.0274 (6) |
| H19 | 0.5775 | 0.6842 | 0.0207 | 0.033* |
| C20 | 0.5869 (4) | 0.64932 (13) | −0.08592 (18) | 0.0342 (6) |
| H20 | 0.7039 | 0.6316 | −0.0714 | 0.041* |
| C21 | 0.4884 (4) | 0.64455 (14) | −0.16209 (18) | 0.0370 (7) |
| H21 | 0.5371 | 0.6231 | −0.2006 | 0.044* |
| C22 | 0.3192 (4) | 0.67099 (12) | −0.18219 (16) | 0.0286 (6) |
| H22 | 0.2511 | 0.6683 | −0.2345 | 0.034* |
| C23 | 1.0929 (4) | 0.93296 (12) | 0.46333 (17) | 0.0319 (6) |
| C24 | 1.2471 (4) | 0.93447 (15) | 0.52810 (18) | 0.0371 (7) |
| H24A | 1.2018 | 0.9298 | 0.5784 | 0.056* |
| H24B | 1.3111 | 0.9706 | 0.5280 | 0.056* |
| H24C | 1.3333 | 0.9040 | 0.5219 | 0.056* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd | 0.01970 (10) | 0.01859 (11) | 0.01415 (10) | −0.00001 (6) | 0.00205 (7) | −0.00045 (6) |
| S1 | 0.0183 (3) | 0.0203 (3) | 0.0206 (3) | 0.0005 (2) | 0.0026 (2) | −0.0025 (2) |
| S2 | 0.0221 (3) | 0.0212 (3) | 0.0254 (3) | 0.0018 (2) | 0.0072 (2) | −0.0035 (2) |
| S3 | 0.0212 (3) | 0.0273 (3) | 0.0199 (3) | −0.0013 (2) | −0.0016 (2) | 0.0036 (2) |
| S4 | 0.0203 (3) | 0.0270 (3) | 0.0190 (3) | −0.0008 (2) | 0.0012 (2) | 0.0055 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1 | 0.0331 (11) | 0.0274 (10) | 0.0200 (9) | −0.0029 (8) | −0.0002 (7) | −0.0002 (7) |
| O2 | 0.0453 (12) | 0.0394 (12) | 0.0185 (9) | 0.0197 (10) | −0.0048 (8) | −0.0023 (8) |
| N1 | 0.0191 (10) | 0.0201 (11) | 0.0160 (9) | 0.0003 (8) | 0.0036 (7) | −0.0002 (7) |
| N2 | 0.0249 (11) | 0.0221 (11) | 0.0173 (10) | 0.0020 (8) | 0.0032 (8) | 0.0022 (8) |
| N3 | 0.0193 (10) | 0.0221 (11) | 0.0201 (10) | −0.0003 (8) | 0.0033 (8) | −0.0016 (8) |
| N4 | 0.0209 (10) | 0.0146 (10) | 0.0177 (10) | 0.0002 (8) | 0.0035 (8) | 0.0016 (7) |
| N5 | 0.0482 (17) | 0.0513 (18) | 0.0362 (14) | −0.0215 (14) | −0.0089 (12) | 0.0155 (12) |
| C1 | 0.0203 (12) | 0.0222 (13) | 0.0122 (10) | 0.0008 (9) | 0.0025 (8) | 0.0015 (8) |
| C2 | 0.0206 (12) | 0.0237 (13) | 0.0200 (11) | −0.0041 (10) | 0.0058 (9) | 0.0008 (9) |
| C3 | 0.0217 (13) | 0.0285 (14) | 0.0244 (13) | −0.0020 (10) | 0.0030 (10) | 0.0030 (10) |
| C4 | 0.0222 (12) | 0.0192 (12) | 0.0174 (11) | −0.0006 (9) | 0.0042 (9) | −0.0033 (9) |
| C5 | 0.0239 (12) | 0.0223 (13) | 0.0190 (11) | 0.0004 (10) | 0.0034 (9) | −0.0016 (9) |
| C6 | 0.0260 (13) | 0.0255 (14) | 0.0287 (13) | 0.0059 (10) | 0.0082 (10) | 0.0010 (10) |
| C7 | 0.0228 (12) | 0.0204 (13) | 0.0161 (11) | 0.0012 (9) | 0.0036 (9) | −0.0015 (9) |
| C8 | 0.0297 (13) | 0.0191 (13) | 0.0191 (11) | 0.0073 (10) | 0.0041 (10) | 0.0011 (9) |
| C9 | 0.0288 (13) | 0.0252 (14) | 0.0184 (11) | 0.0071 (10) | 0.0042 (10) | 0.0003 (9) |
| C10 | 0.0273 (13) | 0.0235 (13) | 0.0202 (11) | −0.0002 (10) | 0.0077 (9) | 0.0021 (9) |
| C11 | 0.0292 (14) | 0.0274 (15) | 0.0317 (14) | −0.0008 (11) | 0.0064 (11) | −0.0028 (11) |
| C12 | 0.0318 (16) | 0.0453 (19) | 0.0338 (15) | −0.0093 (13) | 0.0051 (12) | −0.0038 (13) |
| C13 | 0.0211 (12) | 0.0233 (14) | 0.0234 (12) | 0.0031 (10) | 0.0064 (9) | 0.0023 (9) |
| C14 | 0.0233 (13) | 0.0287 (15) | 0.0273 (13) | 0.0044 (10) | 0.0013 (10) | 0.0061 (10) |
| C15 | 0.0285 (14) | 0.0263 (14) | 0.0227 (13) | −0.0028 (10) | −0.0032 (11) | 0.0037 (10) |
| C16 | 0.0286 (14) | 0.0233 (13) | 0.0166 (11) | −0.0040 (10) | 0.0021 (10) | −0.0001 (9) |
| C17 | 0.0184 (12) | 0.0192 (12) | 0.0167 (11) | −0.0038 (9) | 0.0047 (9) | 0.0006 (9) |
| C18 | 0.0214 (12) | 0.0192 (12) | 0.0180 (11) | −0.0002 (9) | 0.0052 (9) | −0.0007 (9) |
| C19 | 0.0198 (12) | 0.0322 (15) | 0.0293 (13) | 0.0055 (11) | 0.0017 (10) | 0.0006 (11) |
| C20 | 0.0232 (14) | 0.0375 (17) | 0.0433 (17) | 0.0086 (12) | 0.0099 (12) | 0.0007 (13) |
| C21 | 0.0359 (16) | 0.0408 (18) | 0.0381 (16) | 0.0100 (13) | 0.0171 (13) | −0.0078 (13) |
| C22 | 0.0315 (14) | 0.0320 (16) | 0.0238 (13) | 0.0009 (11) | 0.0087 (11) | −0.0069 (11) |
| C23 | 0.0374 (16) | 0.0254 (15) | 0.0330 (15) | −0.0055 (12) | 0.0062 (12) | 0.0069 (11) |
| C24 | 0.0341 (16) | 0.0395 (18) | 0.0361 (16) | 0.0007 (13) | 0.0013 (12) | 0.0090 (13) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cd—N3 | 2.361 (2) | C6—H6B | 0.9800 |
| Cd—N4 | 2.406 (2) | C6—H6C | 0.9800 |
| Cd—S1 | 2.5872 (7) | C8—C9 | 1.515 (3) |
| Cd—S3 | 2.6539 (7) | C8—H8A | 0.9900 |
| Cd—S4 | 2.6704 (7) | C8—H8B | 0.9900 |
| Cd—S2 | 2.7816 (7) | C9—H9A | 0.9900 |
| S1—C1 | 1.736 (2) | C9—H9B | 0.9900 |
| S2—C1 | 1.723 (2) | C10—C11 | 1.527 (4) |
| S3—C7 | 1.723 (3) | C10—H10A | 0.9900 |
| S4—C7 | 1.724 (2) | C10—H10B | 0.9900 |
| O1—C3 | 1.426 (3) | C11—C12 | 1.505 (4) |
| O1—H1O | 0.8400 | C11—H11A | 0.9900 |
| O2—C9 | 1.427 (3) | C11—H11B | 0.9900 |
| O2—H2O | 0.8400 | C12—H12A | 0.9800 |

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|---|---|---|---|
| N1—C1 | 1.340 (3) | C12—H12B | 0.9800 |
| N1—C2 | 1.472 (3) | C12—H12C | 0.9800 |
| N1—C4 | 1.475 (3) | C13—C14 | 1.384 (4) |
| N2—C7 | 1.337 (3) | C13—H13 | 0.9500 |
| N2—C10 | 1.467 (3) | C14—C15 | 1.388 (4) |
| N2—C8 | 1.478 (3) | C14—H14 | 0.9500 |
| N3—C19 | 1.345 (3) | C15—C16 | 1.385 (4) |
| N3—C18 | 1.345 (3) | C15—H15 | 0.9500 |
| N4—C13 | 1.340 (3) | C16—C17 | 1.393 (3) |
| N4—C17 | 1.346 (3) | C16—H16 | 0.9500 |
| N5—C23 | 1.141 (4) | C17—C18 | 1.490 (3) |
| C2—C3 | 1.515 (3) | C18—C22 | 1.395 (3) |
| C2—H2A | 0.9900 | C19—C20 | 1.381 (4) |
| C2—H2B | 0.9900 | C19—H19 | 0.9500 |
| C3—H3A | 0.9900 | C20—C21 | 1.383 (4) |
| C3—H3B | 0.9900 | C20—H20 | 0.9500 |
| C4—C5 | 1.526 (3) | C21—C22 | 1.381 (4) |
| C4—H4A | 0.9900 | C21—H21 | 0.9500 |
| C4—H4B | 0.9900 | C22—H22 | 0.9500 |
| C5—C6 | 1.523 (3) | C23—C24 | 1.443 (4) |
| C5—H5A | 0.9900 | C24—H24A | 0.9800 |
| C5—H5B | 0.9900 | C24—H24B | 0.9800 |
| C6—H6A | 0.9800 | C24—H24C | 0.9800 |

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|---|---|---|---|
| N3—Cd—N4 | 68.37 (7) | S3—C7—S4 | 119.26 (14) |
| N3—Cd—S1 | 141.84 (5) | N2—C8—C9 | 111.5 (2) |
| N4—Cd—S1 | 98.70 (5) | N2—C8—H8A | 109.3 |
| N3—Cd—S3 | 96.53 (5) | C9—C8—H8A | 109.3 |
| N4—Cd—S3 | 143.78 (5) | N2—C8—H8B | 109.3 |
| S1—Cd—S3 | 111.54 (2) | C9—C8—H8B | 109.3 |
| N3—Cd—S4 | 106.87 (5) | H8A—C8—H8B | 108.0 |
| N4—Cd—S4 | 84.70 (5) | O2—C9—C8 | 105.9 (2) |
| S1—Cd—S4 | 107.40 (2) | O2—C9—H9A | 110.5 |
| S3—Cd—S4 | 67.92 (2) | C8—C9—H9A | 110.6 |
| N3—Cd—S2 | 86.66 (5) | O2—C9—H9B | 110.5 |
| N4—Cd—S2 | 118.12 (5) | C8—C9—H9B | 110.5 |
| S1—Cd—S2 | 67.51 (2) | H9A—C9—H9B | 108.7 |
| S3—Cd—S2 | 92.38 (2) | N2—C10—C11 | 112.4 (2) |
| S4—Cd—S2 | 156.855 (19) | N2—C10—H10A | 109.1 |
| C1—S1—Cd | 89.45 (8) | C11—C10—H10A | 109.1 |
| C1—S2—Cd | 83.49 (9) | N2—C10—H10B | 109.1 |
| C7—S3—Cd | 86.69 (8) | C11—C10—H10B | 109.1 |
| C7—S4—Cd | 86.13 (9) | H10A—C10—H10B | 107.9 |
| C3—O1—H1O | 105.4 | C12—C11—C10 | 110.9 (2) |
| C9—O2—H2O | 111.9 | C12—C11—H11A | 109.5 |
| C1—N1—C2 | 122.3 (2) | C10—C11—H11A | 109.5 |
| C1—N1—C4 | 121.6 (2) | C12—C11—H11B | 109.5 |
| C2—N1—C4 | 115.9 (2) | C10—C11—H11B | 109.5 |

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| C7—N2—C10 | 122.5 (2) | H11A—C11—H11B | 108.0 |
| C7—N2—C8 | 121.8 (2) | C11—C12—H12A | 109.5 |
| C10—N2—C8 | 115.6 (2) | C11—C12—H12B | 109.5 |
| C19—N3—C18 | 119.2 (2) | H12A—C12—H12B | 109.5 |
| C19—N3—Cd | 120.38 (17) | C11—C12—H12C | 109.5 |
| C18—N3—Cd | 120.40 (16) | H12A—C12—H12C | 109.5 |
| C13—N4—C17 | 118.6 (2) | H12B—C12—H12C | 109.5 |
| C13—N4—Cd | 122.48 (16) | N4—C13—C14 | 123.0 (2) |
| C17—N4—Cd | 118.74 (16) | N4—C13—H13 | 118.5 |
| N1—C1—S2 | 120.62 (18) | C14—C13—H13 | 118.5 |
| N1—C1—S1 | 119.92 (18) | C13—C14—C15 | 118.4 (2) |
| S2—C1—S1 | 119.46 (14) | C13—C14—H14 | 120.8 |
| N1—C2—C3 | 112.5 (2) | C15—C14—H14 | 120.8 |
| N1—C2—H2A | 109.1 | C16—C15—C14 | 119.2 (2) |
| C3—C2—H2A | 109.1 | C16—C15—H15 | 120.4 |
| N1—C2—H2B | 109.1 | C14—C15—H15 | 120.4 |
| C3—C2—H2B | 109.1 | C15—C16—C17 | 119.0 (2) |
| H2A—C2—H2B | 107.8 | C15—C16—H16 | 120.5 |
| O1—C3—C2 | 108.4 (2) | C17—C16—H16 | 120.5 |
| O1—C3—H3A | 110.0 | N4—C17—C16 | 121.8 (2) |
| C2—C3—H3A | 110.0 | N4—C17—C18 | 116.2 (2) |
| O1—C3—H3B | 110.0 | C16—C17—C18 | 122.0 (2) |
| C2—C3—H3B | 110.0 | N3—C18—C22 | 121.2 (2) |
| H3A—C3—H3B | 108.4 | N3—C18—C17 | 116.2 (2) |
| N1—C4—C5 | 111.54 (19) | C22—C18—C17 | 122.6 (2) |
| N1—C4—H4A | 109.3 | N3—C19—C20 | 122.6 (3) |
| C5—C4—H4A | 109.3 | N3—C19—H19 | 118.7 |
| N1—C4—H4B | 109.3 | C20—C19—H19 | 118.7 |
| C5—C4—H4B | 109.3 | C19—C20—C21 | 118.2 (3) |
| H4A—C4—H4B | 108.0 | C19—C20—H20 | 120.9 |
| C6—C5—C4 | 111.1 (2) | C21—C20—H20 | 120.9 |
| C6—C5—H5A | 109.4 | C22—C21—C20 | 120.0 (3) |
| C4—C5—H5A | 109.4 | C22—C21—H21 | 120.0 |
| C6—C5—H5B | 109.4 | C20—C21—H21 | 120.0 |
| C4—C5—H5B | 109.4 | C21—C22—C18 | 118.8 (3) |
| H5A—C5—H5B | 108.0 | C21—C22—H22 | 120.6 |
| C5—C6—H6A | 109.5 | C18—C22—H22 | 120.6 |
| C5—C6—H6B | 109.5 | N5—C23—C24 | 179.1 (3) |
| H6A—C6—H6B | 109.5 | C23—C24—H24A | 109.5 |
| C5—C6—H6C | 109.5 | C23—C24—H24B | 109.5 |
| H6A—C6—H6C | 109.5 | H24A—C24—H24B | 109.5 |
| H6B—C6—H6C | 109.5 | C23—C24—H24C | 109.5 |
| N2—C7—S3 | 120.65 (19) | H24A—C24—H24C | 109.5 |
| N2—C7—S4 | 120.09 (19) | H24B—C24—H24C | 109.5 |

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| N3—Cd—S1—C1 | −52.88 (11) | Cd—S1—C1—S2 | 3.16 (13) |
| N4—Cd—S1—C1 | −118.76 (9) | C1—N1—C2—C3 | −90.2 (3) |
| S3—Cd—S1—C1 | 81.54 (8) | C4—N1—C2—C3 | 95.2 (3) |

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|---|---|---|---|
| S4—Cd—S1—C1 | 154.10 (8) | N1—C2—C3—O1 | −63.7 (3) |
| S2—Cd—S1—C1 | −1.85 (7) | C1—N1—C4—C5 | −83.9 (3) |
| N3—Cd—S2—C1 | 153.10 (9) | C2—N1—C4—C5 | 90.8 (2) |
| N4—Cd—S2—C1 | 89.84 (9) | N1—C4—C5—C6 | 177.9 (2) |
| S1—Cd—S2—C1 | 1.87 (8) | C10—N2—C7—S3 | 179.42 (18) |
| S3—Cd—S2—C1 | −110.49 (8) | C8—N2—C7—S3 | −3.5 (3) |
| S4—Cd—S2—C1 | −79.80 (9) | C10—N2—C7—S4 | −1.5 (3) |
| N3—Cd—S3—C7 | −105.50 (10) | C8—N2—C7—S4 | 175.58 (18) |
| N4—Cd—S3—C7 | −43.64 (12) | Cd—S3—C7—N2 | 178.9 (2) |
| S1—Cd—S3—C7 | 100.87 (8) | Cd—S3—C7—S4 | −0.15 (14) |
| S4—Cd—S3—C7 | 0.09 (8) | Cd—S4—C7—N2 | −178.9 (2) |
| S2—Cd—S3—C7 | 167.59 (8) | Cd—S4—C7—S3 | 0.15 (13) |
| N3—Cd—S4—C7 | 90.20 (10) | C7—N2—C8—C9 | 91.3 (3) |
| N4—Cd—S4—C7 | 155.69 (10) | C10—N2—C8—C9 | −91.5 (3) |
| S1—Cd—S4—C7 | −106.83 (8) | N2—C8—C9—O2 | −176.7 (2) |
| S3—Cd—S4—C7 | −0.09 (8) | C7—N2—C10—C11 | 89.8 (3) |
| S2—Cd—S4—C7 | −33.49 (10) | C8—N2—C10—C11 | −87.4 (3) |
| N4—Cd—N3—C19 | 178.4 (2) | N2—C10—C11—C12 | 178.6 (2) |
| S1—Cd—N3—C19 | 102.4 (2) | C17—N4—C13—C14 | −0.8 (4) |
| S3—Cd—N3—C19 | −35.7 (2) | Cd—N4—C13—C14 | −175.62 (19) |
| S4—Cd—N3—C19 | −104.5 (2) | N4—C13—C14—C15 | 0.2 (4) |
| S2—Cd—N3—C19 | 56.3 (2) | C13—C14—C15—C16 | −0.2 (4) |
| N4—Cd—N3—C18 | −1.17 (17) | C14—C15—C16—C17 | 0.8 (4) |
| S1—Cd—N3—C18 | −77.2 (2) | C13—N4—C17—C16 | 1.4 (4) |
| S3—Cd—N3—C18 | 144.74 (18) | Cd—N4—C17—C16 | 176.40 (18) |
| S4—Cd—N3—C18 | 75.88 (18) | C13—N4—C17—C18 | −179.0 (2) |
| S2—Cd—N3—C18 | −123.25 (18) | Cd—N4—C17—C18 | −4.0 (3) |
| N3—Cd—N4—C13 | 177.6 (2) | C15—C16—C17—N4 | −1.4 (4) |
| S1—Cd—N4—C13 | −39.79 (19) | C15—C16—C17—C18 | 179.0 (2) |
| S3—Cd—N4—C13 | 107.09 (19) | C19—N3—C18—C22 | 0.9 (4) |
| S4—Cd—N4—C13 | 67.05 (19) | Cd—N3—C18—C22 | −179.6 (2) |
| S2—Cd—N4—C13 | −108.88 (19) | C19—N3—C18—C17 | −179.9 (2) |
| N3—Cd—N4—C17 | 2.78 (17) | Cd—N3—C18—C17 | −0.3 (3) |
| S1—Cd—N4—C17 | 145.43 (16) | N4—C17—C18—N3 | 2.9 (3) |
| S3—Cd—N4—C17 | −67.7 (2) | C16—C17—C18—N3 | −177.5 (2) |
| S4—Cd—N4—C17 | −107.73 (17) | N4—C17—C18—C22 | −177.9 (2) |
| S2—Cd—N4—C17 | 76.34 (18) | C16—C17—C18—C22 | 1.7 (4) |
| C2—N1—C1—S2 | 0.1 (3) | C18—N3—C19—C20 | −1.0 (4) |
| C4—N1—C1—S2 | 174.40 (16) | Cd—N3—C19—C20 | 179.4 (2) |
| C2—N1—C1—S1 | −179.15 (17) | N3—C19—C20—C21 | 0.4 (5) |
| C4—N1—C1—S1 | −4.8 (3) | C19—C20—C21—C22 | 0.5 (5) |
| Cd—S2—C1—N1 | 177.82 (19) | C20—C21—C22—C18 | −0.7 (5) |
| Cd—S2—C1—S1 | −2.96 (12) | N3—C18—C22—C21 | 0.0 (4) |
| Cd—S1—C1—N1 | −177.61 (18) | C17—C18—C22—C21 | −179.2 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1o···N5 | 0.84 | 2.06 | 2.898 (3) | 174 |
| O2—H2o···S2$^{i}$ | 0.84 | 2.55 | 3.388 (2) | 175 |

Symmetry code: (i) *x*, −*y*+3/2, *z*+1/2.